JUMPIN' JUPITER! Metallic Hydrogen

A 1935 theory predicted that hydrogen becomes metallic when enormously intense pressure is applied. But the theory remained unproved for some 60 years until a Lawrence Livermore team tried a "shocking" idea.

The Laboratory's two-stage light-gas gun was instrumental in the shock compression experiments that metallized hydrogen.



YDROGEN is the simplest and most abundant of elements. Composed of abundant of elements. Composed of one proton and one electron, it makes up 90% of our universe (by number of atoms). On Earth, hydrogen is commonly found as a diatomic molecular gas. But on Jupiter, where interior pressure is millions of times greater than that at our planet's surface, the hydrogen molecule is theorized to exist as a superhot liquid metal.

The theory that hydrogen turns metallic under extreme pressure was first advanced in 1935 by Eugene Wigner, who would go on to win a 1963 Nobel Prize in physics for his work in quantum mechanics. Finding experimental evidence of Wigner's hydrogen metallization theory, however, has proven to be extremely difficult for the scientific community. While studies of the universe's lightest material led to discovery of hydrogen's solid and liquid phases, metallic hydrogen remained out of reach until recently.

At Lawrence Livermore National Laboratory, in a series of shock compression experiments funded by Laboratory Directed Research and Development grants, we successfully ended a 60-year search for hard evidence of metallic hydrogen and the precise pressure at which metallization occurs at a particular temperature.

Our success in metallizing hydrogen would not have been achieved without the shock-wave technology built up over more than two decades to support Lawrence Livermore's nuclear weapons program. It represents the integration of the Laboratory's broad capabilities and expertise in gas-gun technology, shock physics, target diagnostics, hydrodynamic computational simulations, cryogenics, and hydrogen and condensed-matter

Knowing what happens when matter, such as hydrogen, encounters enormously high pressure and temperature is critical for the success of the Laboratory's research in areas relevant to our science-based stockpile stewardship mission, such as nuclear explosives, conventional high

explosives, and laser fusion, as well as for our collaborative efforts in planetary science research. For more than two decades, we have been helping improve that understanding through shockcompression studies using our two-stage light-gas gun (see the box on p. 15).

The gas gun permits us to fire hypervelocity projectiles into highly instrumented targets (Figure 1), shocking matter to extreme conditions for a millionth of a second or less. These experiments create pressures of a million-plus atmospheres, temperatures up to thousands of degrees depending upon the material being shocked, and densities several times that of a material's solid state.

In addition to hydrogen, we have performed shock compression experiments on other liquefied gases such as nitrogen, water, carbon dioxide, oxygen, carbon monoxide, deuterium (an isotope of hydrogen), helium, and argon, and on solids such as aluminum, copper, tantalum, and carbon (graphite). Data from such experiments are used to determine a material's equation of state (EOS expresses the relationship between pressure, density, and temperature), to validate theories, and to generate reliable computational models of a material's behavior under a wide range of thermodynamic variables.

Quest for Metallic Hydrogen

Under normal conditions on our planet, molecular hydrogen functions as an insulator, blocking electrical flow. Apply sufficient pressure, theory said, and hydrogen turns metallic, becoming an exceptional conductor of electricity. Theory predicted that metallization would occur when the insulating molecular solid would transform to a metallic monatomic solid at absolute zero—0 degrees kelvin (K) or –460°F. For early metallic hydrogen theorists, "sufficient pressure" was thought to be 0.2 megabars (1 bar is atmospheric pressure at sea level; a megabar, or Mbar, is a million times atmospheric pressure at sea level). Subsequent predictions pushed

metallization pressure to as high as 20 Mbar. At the time our experiments were conducted, the prevailing theory predicted 3 Mbar for solid hydrogen at 0 K.

For 35 years after Wigner proposed his theory, studies on metallic hydrogen were relegated to the theoretical realm because there was no way to approach the subject experimentally. By the 1970s, however, the tools of science had reached a point where it became possible to construct experiments aimed at creating conditions that theory said were required for metallization. At Lawrence Livermore, for example, one research approach² used an explosively driven system that compressed a magnetic field and, in turn, a small sample of hydrogen to megabar pressures without shocking the hydrogen, and thus the temperature of the sample was kept very low. The early Livermore experiments generated pressures similar to those we recently reached (about 2 Mbar). While electrical conductivity was measured, the approach did not provide necessary evidence of metallization; the measurement system was only sensitive to conductivity values much less than that of

In recent years, researchers at other laboratories have attempted to achieve metallization by crushing micrometersized samples of crystalline hydrogen in a diamond anvil cell. This small mechanical press creates very high pressures in a nanogram-sized sample when the small flat faces of two flawless diamonds are forced together, exerting megabar pressure on the sample trapped between them.³ While diamond anvil studies of hydrogen resulted in an initial claim of optical evidence for metallization, this claim was later found to not hold up.4 Significantly, there was no establishment of metallic character using optical probes. Metallic character is most directly established by electrical conductivity measurements, which are not yet possible in diamond anvil cells with hydrogen samples at any pressure.

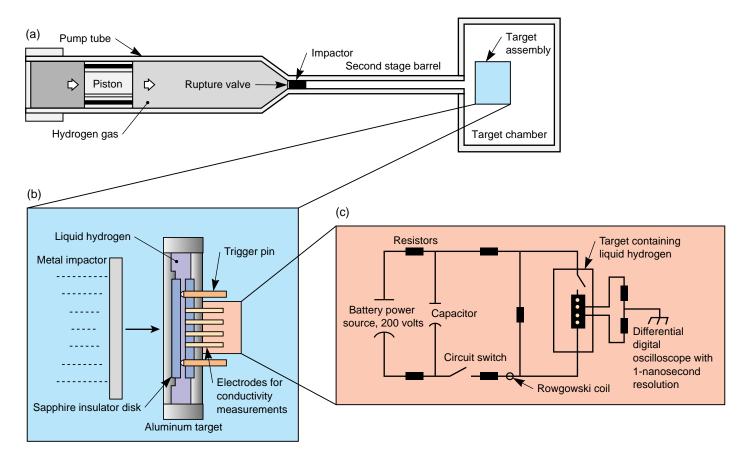


Figure 1. Our success in metallizing hydrogen came during a series of experiments to understand the electrical properties of shocked liquid hydrogen. (a) Our two-stage light-gas gun accelerates plastic-encased aluminum and copper impactor plates to velocities of up to 8 kilometers per second (18,000 mph), sending a shock wave into (b) the target assembly containing a 0.5-millimeter-thick sample of liquid hydrogen. Electrical resistivity/conductivity is measured using (c) a four-probe constant-current circuit. Trigger pins turn on the data-recording equipment when hit by the initial shock wave, and a Rowgowski coil measures current. The circuit is connected to a differential digital oscilloscope, which instantaneously records the electrical quantities during the test.

Our Approach

In 1991, we began a series of experiments to determine how compression affected the electrical properties of diatomic or molecular hydrogen and deuterium both of which are insulators at ambient temperatures and pressures. Our specific objective was to advance fundamental understanding of the way hydrogen transitions from an insulator to a conductor at shock-test pressures and temperatures. Evidence of actual metallization was an unanticipated result of our experiments. It was unexpected for several reasons: (1) we used liquid hydrogen, rather than solid hydrogen that conventional wisdom indicated was required; (2) we applied a methodology-shock compressionthat had never before been tried in order to metallize hydrogen; and (3) we were working at higher

temperatures (3,000 K) than metallization theory specified.

For our experiments, we used liquid hydrogen at an initial temperature of 20 K (-423°F) because: (1) it is easier to liquefy hydrogen than it is to solidify it in our experiments, (2) shock compression dramatically increases temperatures and turns solid hydrogen into liquid, so it made sense to begin with a liquid, and (3) only fluid hydrogen, not solid, is present in highpressure and high-temperature systems that matter to the "real world"-in superhot, hydrogen-rich planets like Jupiter and Saturn and in fusion energy experiments like those conducted at Livermore where laser beams compress tiny spherical targets of liquid deuterium and tritium, both isotopic forms of hydrogen.

As in any shock-wave experiment involving liquids, we confined the liquid hydrogen (or in some cases liquid

How Our Gas Gun Works

Our shock compression studies use a 20-meter-long, twostage light-gas gun built by General Motors in the mid-1960s for ballistic missile studies; the gun has been in operation at the Laboratory since 1972.

The gun consists of a first-stage breech containing up to 3.5 kilograms of gunpowder and a pump tube filled with 60 grams of hydrogen, helium, or nitrogen gas; and a secondstage evacuated barrel for guiding the high-velocity impactor

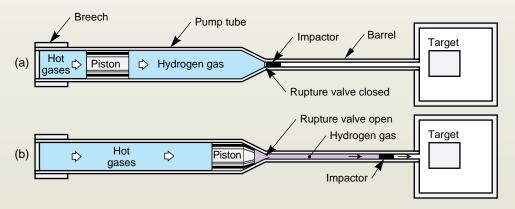
Hot gases from the burning gunpowder drive a heavy (4.5to 6.8-kilograms) piston down the pump tube, compressing the gas. At sufficiently high pressures, the gas eventually breaks a rupture valve and enters the narrow barrel, propelling a 20-gram impactor housed in the barrel toward the target.

When the impactor hits the target, it produces a highpressure shock wave. In a fraction of a microsecond, the

shock wave reverberates through the target. Diagnostic equipment, triggered by the initial wave, measures the properties of the shocked material inside the target during this extremely brief period.

Projectile velocity can range from 1 to 8 kilometers per second (up to 18,000 mph). The preferred velocity is achieved by selecting the appropriate type and amount of gunpowder, driving gas (hydrogen for velocities at or above 4 kilometers per second, helium and nitrogen for lower velocities), pressure required to open the rupture valve, diameter of the barrel, and the metal and mass of the impactor.

The velocity of the shock wave, when combined with the initial conditions (impactor velocity, known densities, equation of state of the projectile and target materials) yields a precise measure of the pressure, density, and energy



(a) In the first stage of the gas gun (blue shading), hot-burning gases from gunpowder drive a piston, which in turn compresses hydrogen gas. (b) In the second stage (pink shading), the highpressure gas eventually ruptures a second-stage valve, accelerating the impactor down the barrel toward its target.

deuterium) in a suitable target container that separated it from the vacuum of the target chamber. (Refer to Figure 1b.) The target walls had the required flat impact surface and were made of a material for which we have an accurate equation of state (aluminum) so that we could compute the pressures, densities, and temperatures reached during the experiments. The liquid hydrogen (or deuterium) was a half millimeter thick, and the target was cryogenically cooled.

We sandwiched the target between two single-crystal sapphire anvils that provide stiffness and electrical

insulation for the four steel electrodes implanted at the surface of the liquid hydrogen inside the target. These electrodes are used to measure the changes in the sample's electrical resistivity/conductivity during shock tests. Two of the electrodes introduce current to the inertially confined hydrogen sample, and two measure voltage across the sample. A trigger pin in the target produces an electrical signal when struck by the initial shock wave, turning on the data recording system (Figure 1c) at the proper moment. The conductivity of the

shocked hydrogen is thus measured before the pressure wave reaches any external surface, that is, before the sample holder blows up when the shock reaches its external surface.

We mounted the anvils on aluminum plates that serve as the front and rear walls of the target, initially at 20 K. At that low temperature, the aluminum remains strong and ductile. Finally, we carefully wrapped the target with 50 layers of aluminized mylar to reduce the heat losses that would boil away the liquid hydrogen and cause our sample to literally

disappear. The impactors aimed at these target samples were made of aluminum and copper embedded in plastic.

Using these impactors in the gas gun, we shocked the hydrogen samples to pressures ranging from 0.9 to 1.8 Mbar and temperatures from 2,000 to 4,000 K. We designed our conductivity experiments to consist of an initial weak shock in the hydrogen followed by a series of very weak shocks reverberating between sapphire anvils, between which our hydrogen sample was sandwiched. In this way, the temperature was kept about ten times lower than it would be for a single sharp shock to the same final pressure. Each data point we recorded using the diagnostics illustrated in Figure 1c represents a measurement taken in about one ten-millionth of a second, which is more than sufficient for the sample to come into equilibrium, that is, reach a stable pressure, density, and temperature. Electrical signal levels of a few hundredths of a volt and currents of about 1 ampere lasted about 200 nanoseconds (200×10^{-9} seconds), indicating that, indeed, metallization had occurred.

Our Results

As shown in Figure 2, we found that from 0.9 to 1.4 Mbar, resistivity in the shocked fluid decreases almost four orders of magnitude (i.e., conductivity increases); from 1.4 to 1.8 Mbar, resistivity is essentially constant at a value typical of that of liquid metals. Our data indicate a continuous transition from a semiconducting to metallic diatomic fluid at 1.4 Mbar, nine-fold compression of initial liquid density, and 3.000 K.

Some theorists have speculated that metallic hydrogen produced under laboratory conditions might remain in that state after the enormous pressures required to create it are removed. However, metallization in our experiments occurred for such a brief period of time, and in such a manner, that questions about hydrogen's superconducting properties and retention of metallic form could not be answered.

At the relatively low temperature, the fluid hydrogen remained almost essentially molecular, rather than breaking into individual atoms. As a

result, electrons in the sample freely flowed from molecule to molecule in a fashion that is characteristic of metals. At metallization, we calculate that only about 5% of the original molecules have separated into individual atoms of hydrogen, which means that our metallic hydrogen is primarily a molecular fluid. (Observation of this molecular metallic state in our experiments was unexpected. Only the monatomic metallic state was predicted by theory.)

In looking at the insulator-to-metal transition, we focused on the changes in electronic energy band-gap (measured in electron volts) in hydrogen under shock compression. The value of the electronic band-gap is the energy that must be absorbed by an electron in order for it to contribute to electrical conduction. A zero band-gap is characteristic of a metal; a positive, nonzero band-gap is characteristic of an insulator. Thus, the magnitude of the band-gap of an insulator is a measure of how far away the insulator is from being a metal.

At ambient pressure, condensed molecular hydrogen has a wide band-gap (about 15 electron volts), making it a

transparent insulator, like glass. Theory said that when hydrogen is squeezed by tremendous pressure, the gap would close to zero (the band-gap of metals, which are nontransparent conductors). Our studies show that when shocked multiple times in a very cold liquid state, hydrogen becomes first a semiconductor and then a fluid metal when, as its density increases, its temperature becomes equal to the band-gap at about 0.3 electron volts (Figure 3). At this point, all the electrons that can be excited by the shock to conduct electricity have been excited. Insensitive to further decreases in band-gap, the conductivity stops changing. Our conductivity data for hydrogen are essentially the same as those for the liquid metals cesium and rubidium at 2,000 K undergoing the same transition from a semiconducting to metallic fluid. The comparison is shown in Figure 4.

Implications/Future Research

Our gas-gun experiments enhance collective knowledge about the interiors of giant planets. Our earlier studies of

temperature measurements of shockcompressed liquid hydrogen led us to conclude that Jupiter's molecular envelope is cooler and has much less temperature variation than previously believed. Further interpretation of those data suggests that there may be no distinct boundary between Jupiter's core and mantle, as there is on Earth.

Jupiter, which is almost 90% hydrogen, is not the only planet rich in metallic hydrogen. Hot metallic hydrogen is believed to make up the interior of Saturn and may be present in other large planets discovered recently outside our solar system. The presence of metallic hydrogen in these planets has a pronounced effect on their behavior. On Jupiter, given its extreme internal pressures, the bulk of hydrogen is most likely in the fluid metallic state; in fact, given the pressure at which hydrogen metallizes, much more metallic hydrogen—the equivalent of 50 times the mass of Earth—exists in Jupiter than previously believed. We also assume this metallic hydrogen is the source of Jupiter's very strong magnetic field, the largest of any planet in our solar system.

The results of our experiments lend credence to the theory that Jupiter's magnetic field is produced not in the core, but close to the Jovian surface (Figure 5). Based on our data, it appears that the band of conductivity producing the magnetic field is much closer to the planet's surface than was thought to be the case.⁷

We anticipate that laser fusion scientists, who use the compressibility of hydrogen to tune laser pulses, also will find the results of our metallic hydrogen experiments extremely useful. Our experiments provide new insight into the behavior of deuterium and tritium, isotopic forms of hydrogen used in laser fusion targets. Higher fusion-energy yields could result from an improved understanding of the temperature-pressure relationship in hydrogen and its isotopes. Indeed, our hydrogen metallization studies suggest strongly that the revised computation of the equation of state of hydrogen at intense pressures will help in perfecting the hydrogen-isotope-filled targets being designed for the National Ignition Facility, making their performance range broader and more flexible. This is also encouraging news for the science-based

Figure 2. As shock compression increases pressure, liquid molecular hydrogen's electrical resistivity falls dramatically, a decrease of almost four orders of magnitude from 0.9 to 1.4 megabars before plateauing between 1.4 and 1.8 megabars where resistivity (and conversely, conductivity) is essentially constant at a value typical of that of a liquid metal. Our experiments used molecular hydrogen and deuterium, which have different densities.

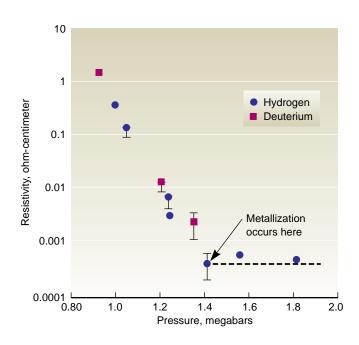


Figure 3. We examined electronic band-gap changes as molecular hydrogen makes the transition from insulator to conductor. At ambient pressure, condensed molecular hydrogen has an electronic energy band-gap of 15 electron volts (eV), making it an excellent insulator. In previous single-shot shock compression experiments (at up to 0.2 megabars pressures and 4,600 degrees kelvin), measurements yielded an energy gap of 11.7 eV.5 The results of our new shock compression studies (shown by the solid part of the curve) indicate that molecular hydrogen becomes metallized when the band-gap is reduced to about 0.3 eV.

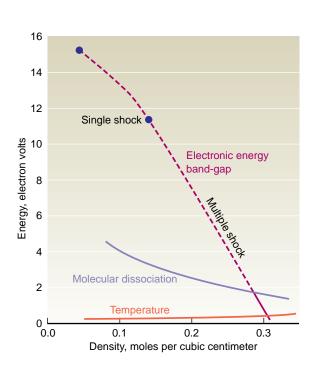
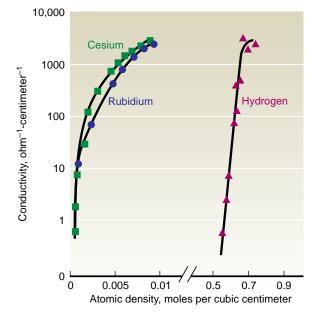
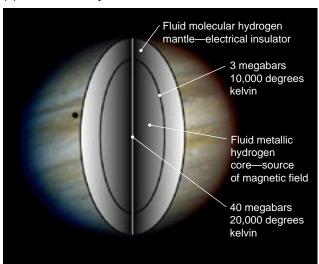


Figure 4. At 2,000 degrees kelvin, conductivity for hydrogen is about the same as that of the metals cesium and rubidium. Liquid molecular hydrogen becomes conducting at a higher density than do those metals.



Science & Technology Review September 1996

(a) Previous theory



(b) Revised theory

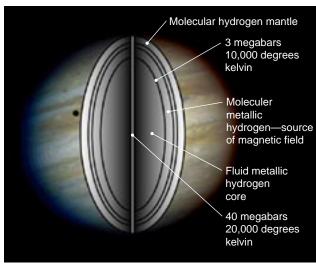


Figure 5. Our work has allowed us to calculate the electrical conductivity in the outer region of Jupiter. The planet's magnetic field is caused by convective dynamo motion of electrically conducting metallic hydrogen. Our results indicate that in Jupiter, the magnetic field is produced much closer to the planet's surface (b) than was thought previously (a).

stockpile stewardship research that will eventually be performed on NIF.

Future experiments will focus on (1) using various hydrogen isotopes—molecular hydrogen, deuterium, and hydrogen—deuterium—to determine the temperature dependence of the electronic energy gap, (2) exploring higher pressures up to 3 Mbar, and (3) probing effects in similar liquids such as molecular nitrogen and argon.

Key Words: gas gun; hydrogen—fluid, liquid, metallic; Jupiter; National Ignition Facility; shock compression tests; stockpile stewardship.

References

- S. T. Weir, A. C. Mitchell, and W. J. Nellis, "Metallization of Fluid Molecular Hydrogen," *Physical Review Letters* 76, 1860 (1996).
- R. S. Hawke, et al., "Observation of Electrical Conductivity of Isentropically Compressed Hydrogen at Mbar Pressures," Physical Review Letters 41, 994 (1978).
- 3. "The Diamond Anvil Cell: Probing the Behavior of Metals under Ultrahigh Pressures," *Science & Technology*

- *Review*, UCRL-52000-3-96 (March 1996), pp. 17–27.
- R. J. Hemley, et al., "Synchrontron Infrared Spectroscopy to 0.15 eV of H₂ and D₂ at Megabar Pressures," Physical Review Letters 76, 1667 (1996) and H. N. Chen, et al., "Extended Infrared Studies of High Pressure Hydrogen," Physical Review Letters 76, 1663 (1996).
- 5. W. J. Nellis, et al., "Electronic Energy Gap of Molecular Hydrogen from Electrical Conductivity Measurements at High Shock Pressures," *Physical Review Letters* **68**, 2937 (1992).
- W. J. Nellis, M. Ross, and N. C. Holmes, "Temperature Measurements of Shock-Compressed Liquid Hydrogen: Implications for the Interior of Jupiter," Science 269, 1249 (1995).
- 7. W. J. Nellis, S. T. Weir, and A. C. Mitchell, "Metallization and Electrical Conductivity of Hydrogen in Jupiter," *Science* (in press).

For further information contact William Nellis (510) 422-7200 (nellis1@llnl.gov).

About the Scientist



Physicist WILLIAM NELLIS joined the Laboratory in 1973. His specialty is the investigation of condensed matter both during and after high-pressure shock compression. The highlight of this work is the observation of the metallization of fluid hydrogen at 1.4 megabars pressure and nine-fold compression. He has delivered invited talks at 44 professional conferences since 1979 and is the author or co-author of more than 100 papers. A fellow of the American Physical Society's Division of Condensed

Matter Physics, Nellis holds M.S. and Ph.D. degrees in physics from Iowa State University. He received his B.S. in physics from Loyola University of Chicago.

Modeling Human Joints and Prosthetic Implants

REPETITIVE motion injuries are one of the fastest growing causes of lost time to business and industry, not to mention their impact on worker health and morale. The orthopedic surgery these injuries sometimes necessitate is costly and painful. The therapy and orthopedic implants associated with degenerative bone and muscle diseases and acute injuries are also costly, and in the case of implants, the initial cost may not be the final cost if and when the implant needs to be replaced.

Computational models of joint anatomy and function can help doctors and physical therapists understand trauma from repetitive stress, degenerative diseases such as osteoarthritis, and acute injuries. Models of prosthetic joint implants can provide surgeons and biomechanical engineers with the analytical tools to improve the life-span of implants and increase patient comfort.¹

With such purposes in mind, the Laboratory embarked about three years ago on a mission to model the whole human hand at high resolution. The challenge is that most biological structures are dauntingly complex, and the hand is no exception. The human wrist alone has eight bones, and the rest of the hand has 19 more, to say nothing of soft tissues—ligaments, tendons, muscles, and nerves—and the interactions among them.

More recently, the Laboratory's Computational Biomechanics Group within the Institute for Scientific Computing Research (ISCR) narrowed the mission to a computational model focusing on the dynamics of specific bones and joints that are often associated with injury or damage. The group also undertook a closely related endeavor: creating a computational model of prosthetic joint implants, initially for the thumb.

In light of the complexity of these models and the need for very high accuracy, it is appropriate that a facility like LLNL—which offers powerful computational resources, an understanding of complex engineering systems, and multidisciplinary expertise—take on these tasks. It is also significant that the work is being done collaboratively through the ISCR and draws on experts from the Laboratory (particularly the Mechanical Engineering Department), academia, medicine, and industry (see the box on p. 20). The

A new prosthetic implant design for the thumb joint. We model the behavior of each design with physiological loads applied. Our technique uniquely reveals regions of high stress (shown in red) versus relatively low stress (blue).

was developed at the Laboratory to address engineering problems involving dynamic deformations, such as the response of bridges to large earthquakes,² is now being used as part of our collaborative joint modeling work.

NIKE3D modeling code, for example, which

Each person's bones differ in shape and size. Our models are based on the detailed anatomy of individual people. We start with high-resolution data obtained from computed tomography or magnetic resonance imaging, as shown in the illustrations on pp. 20–21. Images from a single hand scan involve several gigabytes of raw data, and the models developed from them are highly complex—thus the need for powerful computers.

Focusing on the Hand and Knee

We focused our initial attention on a few joints in the hand. One joint of considerable clinical interest is the thumb carpometacarpal (CMC) joint, which connects the long bone at the base of the thumb with the wrist. During routine grasping activities, CMC joint surfaces are subjected to total forces greater than 200 kilograms (440 pounds), so it is not surprising that injuries are common. The thumb is also often involved in repetitive motion injuries, and the CMC joint is the structure most affected in osteoarthritis, which strikes 8% of the U.S. population. Other joints of considerable interest are the knee and the proximal interphalangeal joint and the metacarpophalangeal joint in the index finger, which have some of the strongest ligaments in the hand.